

Pseudo gap in the density of states in cuprates

Peter Prelovšek and Anton Ramšak

J. Stefan Institute, SI-1000 Ljubljana, Slovenia

Faculty of Mathematics and Physics, University of Ljubljana, SI-1000 Ljubljana, Slovenia

(February 1, 2008)

In the framework of the t - J model for cuprates we analyze the development of a pseudo gap in the density of states (DOS), which at low doping starts to emerge for temperatures $T < J$ and persists up to the optimum doping. The analysis is based on numerical results for spectral functions obtained with the finite-temperature Lanczos method for finite two-dimensional clusters. We find that the pseudo gap scales with J and is robust also in the presence of nearest neighbor repulsive interaction. Numerical results are additionally compared with the self consistent Born approximation (SCBA) results for hole-like (photoemission) and electron-like (inverse photoemission) spectra at $T = 0$. The analysis is suggesting that the origin of the pseudo gap is in short-range antiferromagnetic (AFM) spin correlations and strong asymmetry between the hole and electron spectra in the underdoped regime.

In this paper we present the theoretical analysis of DOS in planar cuprates. As a prototype model we take the standard t - J model, which incorporates strong electron correlations leading to AFM in undoped material and hindered motion of holes in doped system. The emphasis of the present study is on the pseudo gap found in recent angle-resolved photoemission (ARPES) experiments [1] and also in some exact diagonalization studies [2–4]. We add to the model also nearest neighbor repulsion V term,

$$H = -t \sum_{\langle ij \rangle s} (c_{js}^\dagger c_{is} + \text{H.c.}) + \sum_{\langle ij \rangle} [J \mathbf{S}_i \cdot \mathbf{S}_j + (V - \frac{J}{4}) n_i n_j].$$

Here i, j refer to planar sites on a square lattice and c_{is}, c_{is}^\dagger represent projected fermion operators forbidding double occupation of sites.

We study here the planar DOS, defined as $\mathcal{N}(\omega) = 2/N \sum_{\mathbf{k}} A(\mathbf{k}, \omega - \mu)$, where $A(\mathbf{k}, \omega)$ is the electron spectral function [2], and μ denotes the chemical potential. First we calculate the DOS with the finite-temperature Lanczos method [3] for clusters of $N = 18, 20$ sites doped with one hole, $N_h = 1$. Note that $\mathcal{N}^-(\omega)$ corresponds to adding a hole into the system and thus to the photoemission experiments, while $\mathcal{N}^+(\omega)$ represents the inverse photoemission (IPES) spectra.

In Fig. 1 we present $\mathcal{N}(\omega)$ for $J/t = 0.3, 0.6$ [2,4] on a $N = 18$ sites cluster. We note that the pseudo gap scales approximately as $2J$. The analysis at elevated temperatures shows that the gap slowly fills up and disappears at $T \sim J$. The gap remains robust also in the presence of the repulsive V term, which on the other hand suppresses binding of hole pairs. Such an analysis thus suggests that the origin of the pseudo gap is in short-range AFM spin

correlations rather than in the binding tendency of doped holes.

In Fig. 2(a) are shown spectra $\mathcal{N}(\omega)$ obtained on a $N = 20$ sites cluster. We compare these spectra with the DOS within the self-consistent Born approximation [5], obtained in the following manner. We assume that $\mathcal{N}^-(\omega)$ can be approximated with the SCBA *hole* Green's function for adding a hole to an antiferromagnetic reference system [5], Fig. 2(b). $\mathcal{N}^+(\omega)$ can be in SCBA correctly calculated and is presented in Fig. 2(c). The peaks in $\mathcal{N}^+(\omega)$ can well be explained with magnon structure of single hole ground state [6]. As seen in Fig. 2(a) is the total DOS obtained with the SCBA (dashed lines) a reasonable approximation of numerical results.

We conclude stressing that the origin of the pseudo gap found in cuprates seems to be in the short range spin correlations of the reference AFM system, as well as in the strong asymmetry between the hole-like and electron-like spectra in underdoped systems. Namely, $\mathcal{N}^+(\omega)$ should scale linearly with doping c_h but not changing substantially the width and form, while $\mathcal{N}^-(\omega)$ away from chemical potential is less sensitive to c_h . Since μ lies in the pseudo gap, it is plausible that the pseudo gap observable in ARPES should also fill up with c_h , as found in experiments [1].

- [1] Z.-X. Shen and D. S. Dessau, Phys. Rep. **253**, 1 (1995); B. O. Wells *et al.*, Phys. Rev. Lett. **74**, 964 (1995); D. S. Marshall *et al.*, Phys. Rev. Lett. **76**, 4841 (1996); A. Ino *et al.*, Phys. Rev. Lett. **81**, 2124 (1998).
- [2] J. Jaklič and P. Prelovšek, Phys. Rev. B **55**, R7307 (1996); P. Prelovšek, J. Jaklič, and K. Bedell, Phys. Rev. B, (1999).
- [3] For a review, see J. Jaklič and P. Prelovšek, cond-mat/980331 (to appear in Adv. Phys.).
- [4] P. Prelovšek, A. Ramšak, and I. Sega, Phys. Rev. Lett. **81**, 3745 (1998).
- [5] S. Schmitt-Rink, *et al.*, Phys. Rev. Lett. **60**, 2793 (1988); A. Ramšak and P. Prelovšek, Phys. Rev. B **42**, 10415 (1990).
- [6] A. Ramšak and P. Horsch, Phys. Rev. B **48**, 10559 (1993); *ibid.* B **57**, 4308 (1998).

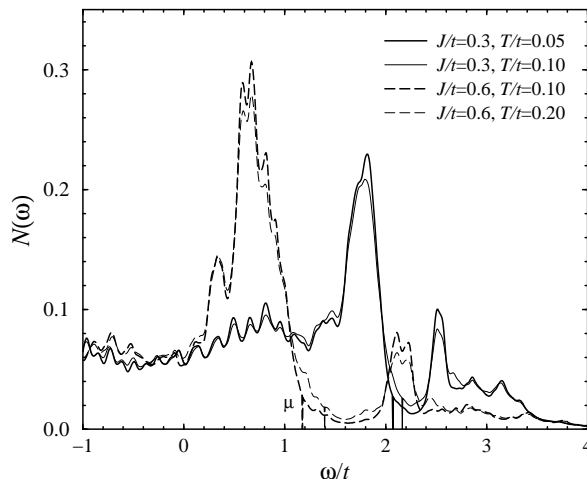


FIG. 1. $\mathcal{N}(\omega)$ for one hole on $N = 18$ sites, presented for different J/t and T/t , at $V = 0$. Broadening of peaks is taken $\epsilon/t = 0.04$.

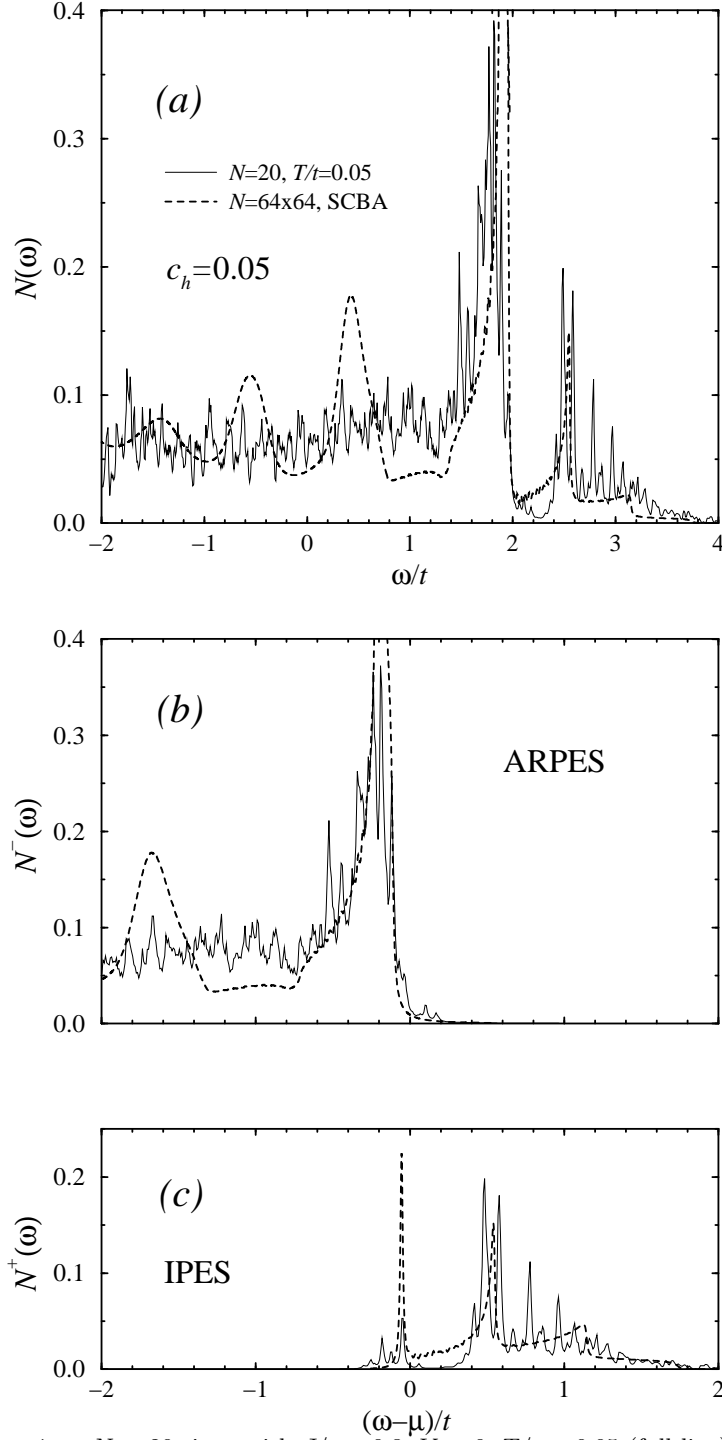


FIG. 2. (a) $N(\omega)$ for $N_h = 1$ on $N = 20$ sites, with $J/t = 0.3$, $V = 0$, $T/t = 0.05$ (full line). Dashed heavy lines represent the SCBA result on large lattice obtained as a sum of $N^-(\omega)$ and $N^+(\omega)$, presented below. (b) Hole-like $N^-(\omega)$ spectra. The SCBA result is obtained on a $N = 64 \times 64$ cluster and for *undoped* reference system. Note the 'string states' resonances, absent in the finite doping Green's function. (c) $N^+(\omega)$ corresponding to IPES. Reference hole concentration is $c_h = 1/N$. The SCBA result is normalized to $c_h = 1/20$. Broadening of peaks is taken $\epsilon/t = 0.01$.